

# Auxiliary quantization constraints on the von Roos ordering-ambiguity at zero binding energies; azimuthally symmetrized cylindrical coordinates

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**Abstract:** Using azimuthally symmetrized cylindrical coordinates, we report the consequences of zero-energy quantal states on the von Roos Hamiltonian. A position-dependent mass  $M(\rho, \varphi, z) = bz^j \rho^{2v+1}/2$  is used. We show that the zero-energy setting not only offers an additional degree of freedom towards feasible separability for the von Roos Hamiltonian, but also manifestly yields auxiliary quantized ambiguity parametric constraints.

## I. INTRODUCTION

Quantum mechanical potentials with zero binding energy (i.e.,  $E = 0$ ) are quantal states that represent (on their own mathematical solvability side) quasi-exactly solvable quantum mechanical systems [1]. Whilst, they form the border line between the continuum and bound states of the energy spectrum, they also offer exact solutions of Schrödinger equation that enlighten quantum-classical correspondence [1–7]. For example, Daboul and Nieto [2–4] have carried out systematic studies on the power-law potentials and found several exceptional normalizable wave functions (i.e., states that do not lie in the continuum spectral region) for  $E = 0$ , where the corresponding states are either bound or unbound. Makowski and Górska [5], have shown that the classical trajectories of a particle precisely match with the localized quantum  $E = 0$  states. Mazharimousavi [7], moreover, have reported the effects of non-Hermitian  $\mathcal{PT}$ -symmetric settings on the localization of the  $E = 0$  states through his study of non-Hermitian quantum-classical correspondence. On their applicability side, however, the  $E = 0$  states are realized applicable in the cold-atom collisions, in the construction of some vortex lattices, in the description of some modes in the Aharonov-Bohm solenoids, and in quantum cosmology (cf, e.g., [5–7] and the related references cited therein).

On the other hand, position-dependent mass (PDM),  $M(\vec{r}) = m_o m(\vec{r})$ , quantum particles are described by the von Roos Hamiltonian [8] (with  $m_o = \hbar = 1$  units)

$$H = -\frac{1}{4} \left[ m(\vec{r})^\gamma \vec{\nabla} m(\vec{r})^\beta \cdot \vec{\nabla} m(\vec{r})^\alpha + m(\vec{r})^\alpha \vec{\nabla} m(\vec{r})^\beta \cdot \vec{\nabla} m(\vec{r})^\gamma \right] + V(\vec{r}), \quad (1)$$

where,  $\alpha$ ,  $\beta$ , and  $\gamma$  are called the von Roos ordering ambiguity parameters satisfying the von Roos constraint  $\alpha + \beta + \gamma = -1$  [8–43]. The ordering ambiguity conflict is obviously manifested by the non-uniqueness representation of the kinetic energy operator (cf., e.g., [19], [33–39]). Nevertheless, in the search for some physically acceptable parametric settings, it is found that the continuity conditions at the abrupt heterojunction between two crystals enforce the condition that  $\alpha = \gamma$  (cf., e.g., Mustafa and Mazharimousavi [19] and Koc et al. [37]). While the parametric proposals of Ben Daniel and Duke ( $\alpha = \gamma = 0$ ,  $\beta = -1$ ), Zhu and Kroemer ( $\alpha = \gamma = -1/2$ ,  $\beta = 0$ ), and Mustafa and Mazharimousavi ( $\alpha = \gamma = -1/4$ ,  $\beta = -1/2$ ) [19] satisfy this condition, the Gora's and Williams' ( $\beta = \gamma = 0$ ,  $\alpha = -1$ ), and Li's and Kuhn's ( $\beta = \gamma = -1/2$ ,  $\alpha = 0$ ) fail to do so. However, even with this ordering ambiguity conflict arising in the process, Lévy-Leblond [40] has advocated the correctness and conceptual consistency of the use of position-dependent mass approximation approach.

In a recent work, Mustafa [41] has considered the von Roos Hamiltonian (1) using cylindrical coordinates and suggested a position-dependent mass that is only radial-dependent (i.e.,  $m(\vec{r}) = m_o M(\rho, \varphi, z) = M(\rho) = 1/\rho^2$ ) in azimuthally symmetrized settings. Later on, Mustafa [42] has offered a parallel azimuthally symmetrized though a rather more general (but still only radially-dependent) power-law-type position-dependent mass (i.e.,  $M(\rho, \varphi, z) = M(\rho) = b\rho^{2v+1}/2$ ). Moreover, spectral signatures of different  $z$ -dependent interaction potential settings on the radial Coulombic and radial harmonic oscillator interaction potentials' spectra were reported.

In the current methodical proposal, our motivation is inspired by a purely theoretical mathematical curiosity as to what consequences would emerge at zero-energy (i.e.,  $E = 0$ ) quantal states for the von Roos Hamiltonian (1). Again, nevertheless, we use cylindrical coordinates in an azimuthally symmetrized setting. We propose a position-dependent mass of yet a more general and mixed dimensional-dependent form  $M(\rho, \varphi, z) = bz^j \rho^{2v+1}/2$ ;  $b, j, v \in \mathbb{R}$ . We show

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that such  $E = 0$  setting not only offers an additional degree of freedom towards feasible separability of Hamiltonian (1), but also manifestly yields quantized ordering ambiguity parametric constraints. To the best of our knowledge, such position-dependent mass settings have not been considered elsewhere.

This work is organized as follows. In section II, we recollect the most relevant and necessary equations of [42] (strictly speaking, equations (2), (4), (5), (6), and (9) of [42] summarized in (2)-(7) below, with  $E = 0$ , of course). In so doing, we make the current work almost self-contained. In the same section, we report on the separability of (1) as a consequence of  $E = 0$  and provide the corresponding components in the 1D-Schrödinger equation format. We show, in section III, that this choice would introduce quantization recipes on the ordering ambiguity parameters. Therein, we give illustrative examples of different interaction potentials that although they may look complicated with mixed coordinates' dependence, their exact solutions are simple and straightforward. The corresponding wave functions are classified as textbook normalizable wave functions. Our concluding remarks are given in section IV.

## II. CYLINDRICAL COORDINATES AT ZERO-ENERGIES AND POWER-LAW PDM

Following closely our recent works [42] on cylindrical coordinates of the PDM-Hamiltonian (1), we again consider the position-dependent mass and the interaction potential to take the forms

$$m(\vec{r}) \equiv M(\rho, \varphi, z) = g(\rho) f(\varphi) k(z) \quad \text{and} \quad V(\vec{r}) \equiv V(\rho, \varphi, z),$$

respectively. We have reported (see Mustafa [42] for more details on this issue) that the corresponding PDM-Schrödinger equation

$$[H - E] \Psi(\rho, \varphi, z) = 0$$

with

$$\Psi(\rho, \varphi, z) = R(\rho) \Phi(\varphi) Z(z); \quad \rho \in (0, \infty), \quad \varphi \in (0, 2\pi), \quad z \in (-\infty, \infty), \quad (2)$$

$$Z(z) = \sqrt{k(z)} \tilde{Z}(z), \quad \Phi(\varphi) = \sqrt{f(\varphi)} \tilde{\Phi}(\varphi), \quad (3)$$

and

$$g(\rho) = \frac{b}{2} \rho^{2v+1}, \quad \text{and} \quad R(\rho) = \rho^v U(\rho), \quad (4)$$

would (with  $E = 0$  in (11) of [42]) imply

$$\begin{aligned} 0 = & \left[ \frac{U''(\rho)}{U(\rho)} + \frac{(2v+1)^2 [\zeta - \beta - 1] - 2v(v+1)}{2\rho^2} - \tilde{V}(\rho) \right] \\ & + \left[ \frac{\tilde{Z}''(z)}{\tilde{Z}(z)} + \frac{(2\zeta-3)}{4} \left( \frac{k'(z)}{k(z)} \right)^2 - \frac{\beta k''(z)}{2 k(z)} - \tilde{V}(z) \right] \\ & + \frac{1}{\rho^2} \left[ \frac{\tilde{\Phi}''(\varphi)}{\tilde{\Phi}(\varphi)} + \frac{(2\zeta-3)}{4} \left( \frac{f'(\varphi)}{f(\varphi)} \right)^2 - \frac{\beta f''(\varphi)}{2 f(\varphi)} - \tilde{V}(\varphi) \right]. \end{aligned} \quad (5)$$

Where

$$\zeta = \alpha(\alpha-1) + \gamma(\gamma-1) - \beta(\beta+1), \quad (6)$$

and

$$2MV(\rho, \varphi, z) = 2g(\rho) f(\varphi) k(z) V(\rho, \varphi, z) = \tilde{V}(\rho) + \tilde{V}(z) + \frac{1}{\rho^2} \tilde{V}(\varphi). \quad (7)$$

Consequently, the zero-energy, assumption secures separability of the von Roos Hamiltonian (1) for some non-zero  $k(z) = z^j$  of  $M(\rho, \varphi, z) = g(\rho) f(\varphi) k(z)$  and hence a more general position-dependent mass form is manifested in the process. That is, our position-dependent mass takes the form (with  $f(\varphi) = 1$ ,  $g(\rho) = b\rho^{2v+1}/2$  and  $k(z) = z^j$ ) as

$$M(\rho, \varphi, z) = bz^j \rho^{2v+1}/2; \quad b, j, v \in \mathbb{R}$$

At this point, one should notice that choosing any other value for  $E$  (i.e.,  $E \neq 0$ ) would make (11) of [42] non-separable under our current methodical proposal settings.

Next, we again choose to remain within azimuthal symmetrization settings and consider that  $\tilde{V}(\varphi) = 0$  and  $f(\varphi) = 1$  in (5) to imply that

$$\frac{\tilde{\Phi}''(\varphi)}{\tilde{\Phi}(\varphi)} = k_\varphi^2 ; k_\varphi^2 = -m^2 ; |m| = 0, 1, 2, \dots, \quad (8)$$

where  $m$  is the magnetic quantum number. Moreover, substituting  $k(z) = z^j$  in (5) yields that

$$\left[ -\partial_z^2 + \tilde{V}(z) + \frac{F(\alpha, \beta, \gamma, j)}{z^2} \right] \tilde{Z}(z) = k_z^2 \tilde{Z}(z), \quad (9)$$

and

$$\left[ -\partial_\rho^2 + \frac{\tilde{\ell}_v^2 - 1/4}{\rho^2} + \tilde{V}(\rho) \right] U(\rho) = -k_z^2 U(\rho), \quad (10)$$

where an irrational magnetic quantum number  $\tilde{\ell}_v$  is introduced in the process as

$$|\tilde{\ell}_v| = \sqrt{v(v+1) + m^2 + \frac{1}{4} - \frac{(2v+1)^2 [\zeta - \beta - 1]}{2}}, \quad (11)$$

and

$$F(\alpha, \beta, \gamma, j) = -j \left[ j \left( \frac{2\zeta - 3}{4} \right) - (j-1) \frac{\beta}{2} \right] \in \mathbb{R}. \quad (12)$$

Hereby,  $F(\alpha, \beta, \gamma, j)/z^2$  plays the role of a manifestly repulsive and/or attractive force field. It is then convenient to use the assumption that

$$F(\alpha, \beta, \gamma, j) = \mathcal{L}^2 - 1/4 \implies \mathcal{L} = \pm \sqrt{F(\alpha, \beta, \gamma, j) + 1/4} \in \mathbb{R} \quad (13)$$

so that the condition

$$F(\alpha, \beta, \gamma, j) + 1/4 \geq 0$$

serves as an auxiliary constraint on the ambiguity parameters. Moreover, our interaction potential takes the general form

$$V(\rho, \varphi, z) = \frac{1}{bz^j \rho^{2v+1}} \left[ \tilde{V}(\rho) + \tilde{V}(z) \right] ; b, j, v \in \mathbb{R}. \quad (14)$$

In the following section, we use simple illustrative examples so that the message of the current methodical proposal is made clear.

### III. $E = 0$ AND AMBIGUITY PARAMETERS' QUANTIZATION CORRESPONDENCE

In this section, we show that when  $E = 0$ , the ordering ambiguity parametric constraints indulge quantization recipes. We use the exactly solvable harmonic oscillator and the Coulomb potentials for constructive illustrations.

A priori, let us provide exact solutions for the  $z$ -dependent equation in (9) by recollecting the exact solutions for the harmonic oscillator,  $\tilde{V}(z) = \tilde{a}^2 z^2/4$ , and for the Coulombic,  $\tilde{V}(z) = -2\tilde{B}/z$ , potentials. In so doing, we shall introduce an impenetrable infinite wall for all  $z < 0$  and hence work in the upper-half of the cylindrical coordinate system at hand. Mathematically speaking, we propose

$$\tilde{V}(z) := \begin{cases} \infty & \text{for } z < 0 \\ \tilde{V}(z) & \text{for } z \geq 0 \end{cases} . \quad (15)$$

Under such settings and in a straightforward manner, one obtains

$$k_z^2 = -\sqrt{\tilde{a}^2} [2n_z + |\mathcal{L}| + 1] \quad (16)$$

for the harmonic oscillator, and

$$k_z = \pm \frac{\tilde{B}}{(n_z + |\mathcal{L}| + 1)} \quad (17)$$

for the Coulombic interaction, where  $\mathcal{L}$  is defined in (13). This would immediately suggest that the corresponding wave functions are also well-known exact solutions. They are, no doubt, the standard textbook normalized wave functions of either the harmonic oscillator or the Coulomb models.

In what follows, the constituents  $\tilde{V}(\rho)$  and  $\tilde{V}(z)$  of the interaction potential  $V(\rho, \varphi, z)$  in (14) shall be chosen to be simple and exactly solvable (Coulombic and/or harmonic oscillator) in their corresponding radial (10) and/or  $z$ -coordinate (9) 1D Schrödinger-like equations. Therefore, the general forms of the corresponding wave functions are exact and textbook normalized wave functions (given by (2) along with (3), and (4)). Four complementary illustrative cases are in order.

**Case 1**  $v = 1/2$ ,  $\tilde{V}(\rho) = a^2 \rho^2/4$ , and  $\tilde{V}(z) = \tilde{a}^2 z^2/4$ .

The substitutions of  $v = 1/2$ ,  $\tilde{V}(\rho) = a^2 \rho^2/4$ , and  $\tilde{V}(z) = \tilde{a}^2 z^2/4$  in (4) and (14) would suggest a position-dependent mass

$$M(\rho, \varphi, z) = bz^j \rho^2/2$$

moving under the influence of an interaction potential

$$V(\rho, \varphi, z) = \frac{a^2}{4bz^j} + \frac{\tilde{a}^2}{4b\rho^2 z^{j-2}}. \quad (18)$$

Hence, the radial equation (10) yields

$$k_z^2 = -\sqrt{a^2} \left[ 2n_\rho + 1 + \sqrt{(m^2 + 3) - 2(\zeta - \beta)} \right], \quad (19)$$

and the  $z$ -dependent equation (9) implies that

$$k_z^2 = \sqrt{\tilde{a}^2} \left[ 2n_z + 1 + \sqrt{F(\alpha, \beta, \gamma, j) + 1/4} \right], \quad (20)$$

where  $F(\alpha, \beta, \gamma, j)$  is given in (12). If we implement an over simplified assumption that  $\sqrt{\tilde{a}^2} = -\sqrt{a^2}$ , one would then use (19) and (20) to obtain

$$-\frac{1}{4} + \left[ 2(n_\rho - n_z) + \sqrt{(m^2 + 3) - 2(\zeta - \beta)} \right]^2 = -j \left[ j \left( \frac{2\zeta - 3}{4} \right) - (j - 1) \frac{\beta}{2} \right]. \quad (21)$$

This is an auxiliary quantization constraint on the ordering ambiguity parameters.

**Case 2**  $v = -1$ ,  $\tilde{V}(\rho) = -2\tilde{A}/\rho$ , and  $\tilde{V}(z) = \tilde{a}^2 z^2/4$

Such proposals in (4) and (14) would imply a position-dependent mass

$$M(\rho, \varphi, z) = bz^j \rho^{-1}/2$$

moving in an interaction potential of the form

$$V(\rho, \varphi, z) = -\frac{2\tilde{A}}{bz^j} + \frac{\tilde{a}^2 \rho}{4bz^{j-2}}. \quad (22)$$

In this case, the radial equation (10) yields

$$k_z = \pm \frac{\tilde{A}}{\left( n_\rho + 1 + \sqrt{(m^2 + 3/4) - (\zeta - \beta)/2} \right)}, \quad (23)$$

and the  $z$ -dependent equation (9) gives

$$k_z^2 = \sqrt{\tilde{a}^2} \left[ 2n_z + 1 + \sqrt{F(\alpha, \beta, \gamma, j) + 1/4} \right]. \quad (24)$$

Therefore,

$$-\frac{1}{4} + \left[ \frac{\tilde{A}^2 / |\tilde{a}|}{\left( n_\rho + 1 + \sqrt{(m^2 + \frac{3}{4}) - \frac{(\zeta - \beta)}{2}} \right)^2} - 2n_z - 1 \right]^2 = -j \left[ j \left( \frac{2\zeta - 3}{4} \right) - (j - 1) \frac{\beta}{2} \right]. \quad (25)$$

Which is now the auxiliary quantization constraint on the ambiguity parameters.

**Case 3**  $v = 1/2$ ,  $\tilde{V}(\rho) = a^2 \rho^2 / 4$ , and  $\tilde{V}(z) = -2\tilde{B}/z$

Such model suggests a position-dependent mass

$$M(\rho, \varphi, z) = bz^j \rho^2 / 2$$

moving in an interaction potential of the form

$$V(\rho, \varphi, z) = \frac{a^2}{4bz^j} - \frac{2\tilde{B}}{b\rho^2 z^{j+1}}. \quad (26)$$

Therefore,

$$k_z = \pm |a| \left[ 2n_\rho + 1 + \sqrt{(m^2 + 3) - 2(\zeta - \beta)} \right]^{1/2}, \quad (27)$$

$$k_z = \pm \frac{\tilde{B}}{\left( n_z + 1 + \sqrt{F(\alpha, \beta, \gamma, j) + 1/4} \right)}, \quad (28)$$

and the auxiliary quantization constraint on the ambiguity parameters reads

$$-\frac{1}{4} + \left[ \frac{\tilde{B} / |a|}{\left( 2n_\rho + 1 + \sqrt{(m^2 + \frac{3}{4}) - \frac{(\zeta - \beta)}{2}} \right)^{\frac{1}{2}}} - n_z - 1 \right]^2 = -j \left[ j \left( \frac{2\zeta - 3}{4} \right) - (j - 1) \frac{\beta}{2} \right]. \quad (29)$$

**Case 4**  $v = -1$ ,  $\tilde{V}(\rho) = -2\tilde{A}/\rho$ , and  $\tilde{V}(z) = -2\tilde{B}/z$

This yields a position-dependent mass of the form

$$M(\rho, \varphi, z) = bz^j \rho^{-1} / 2$$

and an interaction potential

$$V(\rho, \varphi, z) = -\frac{2\tilde{A}}{bz^j} - \frac{2\tilde{B}\rho}{bz^{j+1}}. \quad (30)$$

Hence,

$$k_z = \pm \frac{\tilde{A}}{\left( n_\rho + 1 + \sqrt{(m^2 + 3/4) - (\zeta - \beta)/2} \right)}, \quad (31)$$

$$k_z = \pm \frac{\tilde{B}}{\left( n_z + 1 + \sqrt{F(\alpha, \beta, \gamma, j) + 1/4} \right)}, \quad (32)$$

and the auxiliary quantization constraint on the ambiguity parameters is

$$-\frac{1}{4} + \left[ \frac{\tilde{B}}{\tilde{A}} \left( n_\rho + 1 + \sqrt{\left( m^2 + \frac{3}{4} \right) - \frac{(\zeta - \beta)}{2}} \right) - n_z - 1 \right]^2 = -j \left[ j \left( \frac{2\zeta - 3}{4} \right) - (j - 1) \frac{\beta}{2} \right]. \quad (33)$$

In the four cases discussed above, we observe auxiliary quantization constraints on the ordering ambiguity parameters (documented in the appearance of  $n_\rho$ ,  $n_z$ , and  $m$  quantum numbers in (21), (25), (29), and (33)). That is, for each set of values of  $n_\rho$ ,  $n_z$ , and  $m$  there is a corresponding quantized ordering ambiguity parametric constraint. For example, in Case 1 and for  $j = 0$  in (21), one obtains  $F(\alpha, \beta, \gamma, j) = 0$  and

$$\zeta - \beta = \frac{1}{2} \left[ m^2 + 3 - \left( 2n_z - 2n_\rho + \frac{1}{2} \right)^2 \right], \quad (34)$$

where  $\zeta$  is given in (6). It is obvious here that for every set of values of  $n_\rho$ ,  $n_z$ , and  $m$  the profile of the ordering ambiguity parameters would change and consequently the profile of the kinetic energy operator in (1) would change. Hence the effective potential of (1) would change its profile too. Moreover, one observes that for  $n_\rho = n_z = |m| = 0$ , this quantized constraint (34) is only satisfied by the set of  $\alpha = \gamma = -1/4$  and  $\beta = -1/2$  of Mustafa and Mazharimousavi [19]. Such a result does not make this parametric set as a universally acceptable one, of course. Changing the quantum numbers  $n_\rho$ ,  $n_z$ , and  $m$  would change the profile of the acceptable parametric sets. The same trend may very well be observed in Cases 2, 3, and 4. The ordering ambiguity constraints' quantization correspondence, as an obvious manifestation of  $E = 0$  quantal states, is therefore clear.

#### IV. CONCLUDING REMARKS

Under azimuthally symmetric settings, we have recollected the most relevant and vital relations (equations (2)-(7) above) that have been readily reported by Mustafa [42] for cylindrical coordinates separability of the von Roos Hamiltonian (1). Therein [42], the position-dependent mass  $M(\rho, \varphi, z) = g(\rho) = b\rho^{2v+1}/2$ ;  $v, b \in \mathbb{R}$  is introduced as a generalization of  $M(\rho, \varphi, z) = g(\rho) = 1/\rho^2$  of [41]. Spectral signatures of different  $z$ -dependent interaction potential settings on the radial Coulombic and radial harmonic oscillator interaction potentials' spectra were reported.

In the current methodical proposal, however, we have discussed the consequences of choosing zero-energy states (i.e., states with  $E = 0$ ) for our position-dependent mass Hamiltonian (1) under azimuthally symmetrized cylindrical coordinates settings. Moreover, we have used a more general position-dependent mass function,  $M(\rho, \varphi, z) = bz^j\rho^{2v+1}/2$ ;  $b, j, v \in \mathbb{R}$ . We have shown that the choice of  $E = 0$  setting provides not only an additional degree of freedom towards the feasible separability of Hamiltonian (1), but also manifestly yields quantized ordering ambiguity parametric constraints (documented in (21), (25), (29), (33), and (34)). We have also shown that even with the simplistic choices of the constituent interaction potentials  $\tilde{V}(\rho)$  and  $\tilde{V}(z)$ , the overall general interaction potentials,  $V(\rho, \varphi, z)$ , turned out to be complicated in the sense of indulging mixed coordinates dependence (documented in (18), (22), (26), and (30)). Yet, their exact solutions are simple and straightforward. They are the exact and textbook normalizable wave functions of either the harmonic oscillator or the Coulomb models in (9) and (10). Consequently, the overall general forms of the wave functions are exact, textbook normalizable, and given through (2), (3), and (4).

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